

Hyperspherical three-body model calculation for the bound $1,3S$ -states of Coulombic systems

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Abstract

In this paper, hyperspherical three-body model formalism has been applied for the calculation energies of the low-lying bound $1,3S$ ($L=0$)-states of neutral helium and helium like Coulombic three-body systems having nuclear charge (Z) in the range $Z=2$ to $Z=92$. The calculation of the coupling potential matrix elements of the two-body potentials has been simplified by the introduction of Raynal-Revai Coefficients (RRC). The three-body wave function in the Schrödinger equation when expanded in terms of hyperspherical harmonics (HH), leads to an infinite set of coupled differential equation (CDE). For practical reason the infinite set of CDE is truncated to a finite set and are solved by an exact numerical method known as renormalized Numerov method (RNM) to get the energy solution (E). The calculated energy is compared with the ones of the literature.

Keywords: Raynal Revai Coefficient, Hyperspherical Harmonics, Coupled Differential Equation, Potential Matrix Elements, Renormalized Numerov Method.

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1 Introduction

In physics, role of few-body (two- or three-body) problems are very important for the proper understanding of the physics underlying the internal configurations and kinematics of more complex many-body systems, usually made of interacting bosons and (or) fermions. As few-body systems are the building blocks of more complex many-body systems, they are important not only in nuclear, particle, plasma, astro-nuclear or hyper-nuclear physics but in atomic physics as well. For example, the lightest few-body systems like neutral helium atom and helium-like ions have long history as subject of attraction for both theoretical and experimental investigations. These atomic systems constituting the simplest few-body problems in atomic physics are traditionally used as testing ground for different methods of description of the structure of atoms. On the experimental side, small natural line widths of transition among

various metastable quantum states of helium-like systems allow spectroscopic measurements of very high precision. In addition, few-body systems made up of electrons, protons, muons, deuteron, kaon etc. and their antimatters are found to be of strong interest in many areas of physics including atomic spectroscopy, quantum electrodynamics, particle physics and astrophysics [1-2]. In recent years, highly ionized atoms are being studied extensively to explain the origin of X-rays spectra from the solar corona and other astrophysical plasmas. It is worth mentioning here that highly ionized atoms can be produced in the laboratory by collision of ions with atoms or directing energetic projectile beams towards matter foils and their spectra can also be studied in the laboratory.

A number of theoretical methods have been adopted to investigate the bound state properties of atomic few-body systems. For example, we may refer the works of Lin [3-5], Lin et al [6] in which the author(s) has (have) applied hyperspherical coordinates to Coulombic three-body systems to calculate channel potential, channel function, binding energies and some other observables of the systems. Huang [7] investigated muonic helium atom as a three-body problem in correlated wave function approach. Some more works which may be referred here include those found in references [8-17]. Rajaraman et al [18] presented results of three-body problems originated in the nuclear matter. Alexander et al [19] reported analytical results for the trimmer binding energies and other three-body parameters considering three-body system of identical bosonic atoms. Frolov [20] adopted exponential expansion based variational approach to construct highly accurate wave functions for the triplet spin states of helium like two-electron ions like Li^+ (atomic number $Z=3$) to Ne^{8+} (atomic number $Z=10$). The ground state properties of some two-electron and electron-muon atomic three-body systems has been studied by Rodriguez et al [21] applying the Angular Correlated Configuration Interaction (ACCI) approach. The calculated energy for negatively charged hydrogen-like systems; neutral helium-like systems, and positively charged lithium like systems. However, more accurate results for these systems are reported by Smith Jr et al [22], Frolov et al [23-31], Thakkar and Koga [32], Goldman [33], Korobov [34] and Drake [35]. Researchers like- Hylleraas and Ore [36], Hill [37], Mohr and Taylor [38], Drake, Cassar and Razvan [39], Frolov [40], Mills [41-42], Ho [43-44] and Wen-Fang [45] have explored the bound state properties of exotic positronium negative ion $Ps^-(e^+e^-e^-)$. Ancarani et al [1-2] also reported the ground and excited state energies for several three-body atomic systems obtained by applying ACCI approach. Kubicek et al [46] and Kondrashev et al [47] conducted experiments on production of He-like ions. In this paper we present energies of the low-lying bound $1,3S$ -states of neutral helium and helium like two-electron Coulombic three-body systems having nuclear charge number Z in the range $Z=2 - 92$. The resulting three-body Schrödinger equation has been solved in the framework of hyperspherical harmonics expansion (HHE) formalism applying an exact numerical method known as renormalized Numerov method (RNM) [48]. The scheme of solution of the three-body Schrödinger equation in HHE approach has been described in more details in our earlier works [49-62]. In HHE approach for a general three-body system containing particles of arbitrary masses, there are three possible partitions and in the i^{th} partition, the particle labeled i , acts as a spectator while the remaining two, labeled j and k form the interacting pair. For the calculation matrix element of the potential of the (jk) pair, $V(r_{jk})$, it is convenient to expand the chosen HH in the set of HH corresponding to the par-

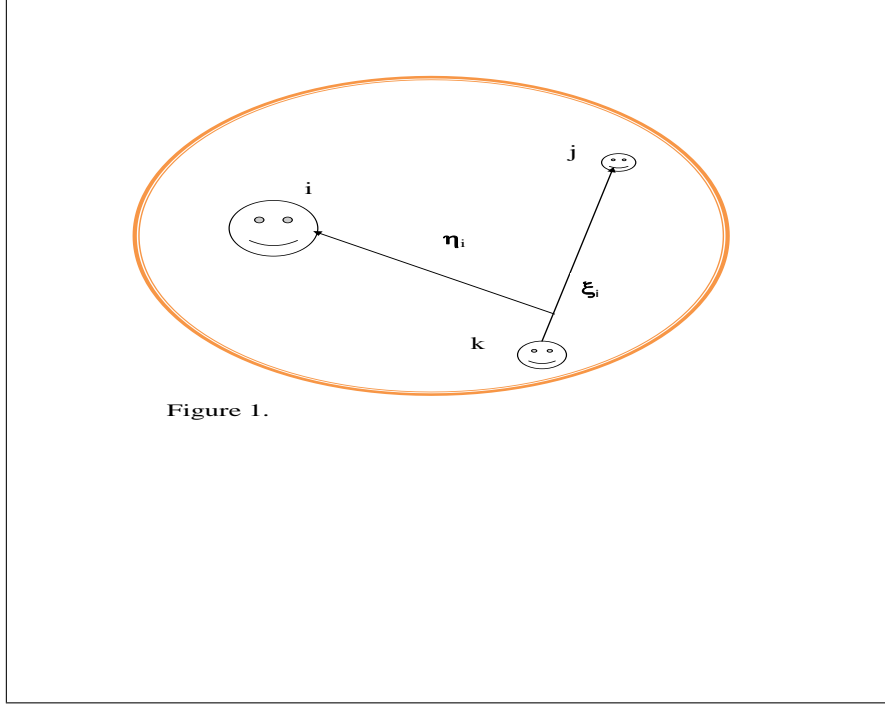


Figure 1.

Figure 1: Particle label scheme for general three-body system and choice of Jacobi coordinates in the i^{th} partition.

tition in which the potential r_{jk}^{-1} is proportional to the first Jacobi vector $\vec{\xi}_i$ [49] and this has been done using Raynal-Revai coefficients (RRC) [63]. In the numerical procedure of computation of potential matrix elements of the two-body potentials involved in the system of three particles constituted by a relatively heavy and positively charged nucleus being orbited by two valence electrons, we used RRC of [49,64]. The energies of the low-lying bound $1,3S$ -states of several Coulombic three-body systems obtained by solving the three-body Schrödinger equation have been compared with the ones of the literature.

In Section 2, we will give a very concise description of the HHE method along with the scheme of transformation between two sets of HH which correspond to two different partitions. In Section 3, we will discuss the application of HHE to the low-lying bound spin singlet (spin $S=0$) and spin triplet (spin $S=1$) i.e. $1,3S$ ($L=0$)-states of neutral helium and similar other systems to calculate the energies and compare them with the ones of the literature.

2 HHE Method

In the hyperspherical harmonics expansion (HHE) method for a general three-body system of particles of arbitrary masses m_i, m_j, m_k as depicted in Figure 1, the Jacobi coordinates [64] in the partition - " i " are defined as

$$\left. \begin{aligned} \vec{\xi}_i &= \left[\frac{m_j m_k M}{m_i (m_j + m_k)^2} \right]^{\frac{1}{4}} (\vec{r}_j - \vec{r}_k) \\ \vec{\eta}_i &= \left[\frac{m_i (m_j + m_k)^2}{m_j m_k M} \right]^{\frac{1}{4}} \left(\vec{r}_i - \frac{m_j \vec{r}_j + m_k \vec{r}_k}{m_j + m_k} \right) \end{aligned} \right\} \quad (1)$$

where $M = m_i + m_j + m_k$ and the condition that (i, j, k) should form a cyclic permutation of $(1, 2, 3)$ determines the sign of $\vec{\xi}_i$.

The set of Jacobi coordinates represented by eq.(1) above corresponds to the partition, in which, the particle labeled “ i ” is the spectator and the remaining particles labeled “ j ” and “ k ” form the interacting pair. The reason behind such nomenclature is that the calculation of matrix element of $V(\vec{r}_{jk})$ in terms of the above set of Jacobi coordinates is straight forward. In the similar manner, we can also define two other sets of Jacobi coordinates by cyclically permuting $i \rightarrow j \rightarrow k \rightarrow i$ twice, which correspond to j^{th} and k^{th} partitions respectively. In hyper-spherical variables [65-66] of the i^{th} partition, three-body Schrödinger equation is

$$\left[-\frac{\hbar^2}{2\mu\rho^5} \frac{\partial}{\partial\rho} (\rho^5 \frac{\partial}{\partial\rho}) + \frac{\hbar^2}{2\mu\rho^2} \frac{\hat{\mathcal{N}}^2(\Omega_i)}{\rho^2} + V(\rho, \Omega_i) - E \right] \Psi(\rho, \Omega_i) = 0 \quad (2)$$

where $\mu = \left[\frac{m_i m_j m_k}{M} \right]^{\frac{1}{2}}$ is an effective mass parameter, $V(\rho, \Omega_i) = V_{jk} + V_{ki} + V_{ij}$ is the total interaction potential, and $\hat{\mathcal{N}}^2(\Omega_i)$ is the square of the hyper angular momentum operator satisfying the eigenvalue equation [67]

$$\hat{\mathcal{N}}^2(\Omega_i) \mathcal{H}_{N\alpha_i}(\Omega_i) = N(N+4) \mathcal{H}_{N\alpha_i}(\Omega_i) \quad (3)$$

where

$$\begin{aligned} \mathcal{H}_{N\alpha_i}(\Omega_i) &\equiv \mathcal{H}_{Nl_{\xi_i}l_{\eta_i}LM}(\phi_i, \theta_{\xi_i}, \phi_{\xi_i}, \theta_{\eta_i}, \phi_{\eta_i}) \\ &\equiv {}^{(2)}P_N^{l_{\xi_i}l_{\eta_i}}(\phi_i) \left[Y_{l_{\xi_i}m_{\xi_i}}(\theta_{\xi_i}, \phi_{\xi_i}) Y_{l_{\eta_i}m_{\eta_i}}(\theta_{\eta_i}, \phi_{\eta_i}) \right]_{LM} \end{aligned} \quad (4)$$

is the normalized eigenfunction known as hyperspherical harmonics (HH), L is the total orbital angular momentum of the system with M as its projection, $\Omega_i \rightarrow \{\phi_i, \theta_{\xi_i}, \phi_{\xi_i}, \theta_{\eta_i}, \phi_{\eta_i}\}$, $\alpha_i \equiv \{l_{\xi_i}, l_{\eta_i}, L, M\}$ is a short hand notation and $[\]_{LM}$ indicates angular momentum coupling. The quantity $N = 2n_i + l_{\xi_i} + l_{\eta_i}$ (n_i being a non-negative integer) is the hyper-angular momentum quantum number which is not a good quantum number for the three-body system. In terms of HH associated with a given partition, (say partition “ i ”), the wave-function $\Psi(\rho, \Omega_i)$ is expanded in the complete set of HH

$$\Psi(\rho, \Omega_i) = \sum_{N\alpha_i} \frac{U_{N\alpha_i}(\rho)}{\rho^{5/2}} \mathcal{H}_{N\alpha_i}(\Omega_i) \quad (5)$$

Substitution of eq.(5) in eq.(2), use of eq.(3) and the ortho-normality of HH, leads to a set of coupled differential equations (CDE) in ρ

$$\begin{aligned} &\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{d\rho^2} + \frac{\hbar^2}{2\mu} \frac{(N+3/2)(N+5/2)}{\rho^2} - E \right] U_{N\alpha_i}(\rho) \\ &+ \sum_{N'\alpha'_i} \langle N'\alpha'_i | V(\rho, \Omega_i) | N\alpha_i \rangle U_{N'\alpha'_i}(\rho) = 0. \end{aligned} \quad (6)$$

where

$$\langle N\alpha_i | V | N', \alpha'_i \rangle = \int \mathcal{H}_{N\alpha_i}^*(\Omega_i) V(\rho, \Omega_i) \mathcal{H}_{N'\alpha'_i}(\Omega_i) d\Omega_i \quad (7)$$

For central potentials, computation of the matrix elements of the form

$$\langle \mathcal{H}_{N\alpha_i}(\Omega_i) | V_{jk}(\xi_i) | \mathcal{H}_{N'\alpha'_i}(\Omega_i) \rangle$$

is straight forward, while for matrix elements of the forms

$$\langle \mathcal{H}_{N\alpha_i}(\Omega_i) | V_{ki}(\xi_j) | \mathcal{H}_{N'\alpha'_i}(\Omega_i) \rangle$$

or

$$\langle \mathcal{H}_{N\alpha_i}(\Omega_i) | V_{ij}(\xi_k) | \mathcal{H}_{N'\alpha'_i}(\Omega_i) \rangle$$

computations become very complicated even for central potentials. This is because the vectors $\vec{\xi}_j$ or $\vec{\xi}_k$ depend on the polar angles of the vectors $\vec{\xi}_i$ and $\vec{\eta}_i$. Vectors $\vec{\xi}_k$ and $\vec{\eta}_k$ can be expressed in terms of $\vec{\xi}_i$ and $\vec{\eta}_i$ using eq.(1) as

$$\left. \begin{aligned} \vec{\xi}_k &= -\cos \sigma_{ki} \vec{\xi}_i + \sin \sigma_{ki} \vec{\eta}_i \\ \vec{\eta}_k &= -\sin \sigma_{ki} \vec{\xi}_i - \cos \sigma_{ki} \vec{\eta}_i \end{aligned} \right\} \quad (8)$$

where $\sigma_{ki} = \tan^{-1}\{(-1)^P \sqrt{\frac{Mm_j}{m_i m_k}}\}$, P being even (odd) if (kij) is an even (odd) permutation of the triad (1 2 3). Now for any arbitrary shape of the central potential with non-vanishing L, most of the five dimensional integrals have to be done numerically which makes the calculation time consuming and inaccurate. However computation of the latter matrix elements can be greatly simplified using the following prescription. At first it is to be noted that each of the complete sets of HH $\{\mathcal{H}_{N\alpha_i}(\Omega_i)\}$, $\{\mathcal{H}_{N\alpha_j}(\Omega_j)\}$ or $\{\mathcal{H}_{N\alpha_k}(\Omega_k)\}$ span the same five dimensional angular hyperspace. Then a particular member of a given set, say $\mathcal{H}_{N\alpha_i}(\Omega_i)$ can be expanded in the complete set of $\{\mathcal{H}_{N\alpha_k}(\Omega_k)\}$ through a unitary transformation:

$$\mathcal{H}_{N\alpha_i}(\Omega_i) = \sum_{\alpha_k} \langle \alpha_k | \alpha_i \rangle_{NL} \mathcal{H}_{N\alpha_k}(\Omega_k) \quad (9)$$

As N, L, M are conserved for eq.(9) and there is rotational degeneracy with respect to the quantum number M for spin independent forces, we have

$$\langle \alpha_k | \alpha_i \rangle_{NL} = \langle l_{\xi_k} l_{\eta_k} | l_{\xi_i} l_{\eta_i} \rangle_{NL} \quad (10)$$

Thus, eq.(9) can be rewritten as [52]

$$\mathcal{H}_{N\alpha_i}(\Omega_i) = \sum_{l_{\xi_k} l_{\eta_k}} \langle l_{\xi_k} l_{\eta_k} | l_{\xi_i} l_{\eta_i} \rangle_{NL} \mathcal{H}_{N\alpha_k}(\Omega_k) \quad (11)$$

The coefficients involved in eq.(10) and (11) are called the Raynal-Revai Coefficients (RRC) and these are independent of M due to overall rotational degeneracy. In terms of these coefficients, the matrix element of a central interaction V_{ij} then becomes

$$\begin{aligned} & \langle \mathcal{H}_{N\alpha_i}(\Omega_i) | V_{ij}(\xi_k) | \mathcal{H}_{N'\alpha'_i}(\Omega_i) \rangle \\ &= \sum_{l'_{\xi_k} l'_{\eta_k}} \langle l_{\xi_k} l_{\eta_k} | l_{\xi_i} l_{\eta_i} \rangle_{NL}^* \times \langle l'_{\xi_k} l'_{\eta_k} | l'_{\xi_i} l'_{\eta_i} \rangle_{N'L} \\ &\times \langle \mathcal{H}_{N\alpha_k}(\Omega_k) | V_{ij}(\xi_k) | \mathcal{H}_{N'\alpha'_k}(\Omega_k) \rangle \end{aligned} \quad (12)$$

The matrix element on the right side of eq.(12) has the same form as the matrix element of V_{jk} in the partition i and can be calculated in a straight forward manner. Thus computing the values of RRC's involved in eq.(12) using their explicit expressions found in [49, 63], one can calculate the matrix element of V_{ij} easily. Similar prescription can also be employed for the calculation of the matrix element of V_{ki} .

3 Application to Coulombic three-body systems

We apply the scheme of RRC to the low-lying bound $^1,^3\text{S}$ ($L=0$)-states of Coulombic three-body system containing relatively massive and positively charged nuclear core plus two extra core orbital electrons. We label the nuclear core having mass m_C and charge $+Ze$ as the i^{th} particle, two electrons of mass $m_j = m_k = m$ and charge $-e$ as the j^{th} and k^{th} particles respectively. For this particular choice mass of the system particles, Jacobi coordinates of eq.(1) in corresponding to the partition i becomes

$$\left. \begin{aligned} \vec{\xi}_i &= \beta_i(\vec{r}_j - \vec{r}_k) \\ \vec{\eta}_i &= \frac{1}{\beta_i}(\vec{r}_i - \frac{\vec{r}_j + \vec{r}_k}{2}) \end{aligned} \right\} \quad (13)$$

where the dimensionless parameter $\beta_i = \left[\frac{m_C + 2m}{4m_C} \right]^{\frac{1}{4}}$ can be connected to the effective mass μ as

$$\mu = m \left(\frac{m_C}{m_C + 2m} \right)^{\frac{1}{2}} = \frac{m}{2\beta_i^2} \quad (14)$$

In atomic unit (ie., $\hbar^2 = m = e^2 = 1$), eq.(6) becomes

$$\left. \begin{aligned} &\left[-\beta_i^2 \frac{d^2}{d\rho^2} + \beta_i^2 \frac{(N+3/2)(N+5/2)}{\rho^2} - E \right] U_{N\alpha_i}(\rho) \\ &+ \sum_{N'\alpha'_i < N\alpha_i} \left| \frac{\beta_i}{\rho \cos \phi_i} - \frac{Z}{\rho |(\beta_i \sin \phi_i) \hat{\eta}_i - (\frac{1}{2\beta_i} \cos \phi_i) \hat{\xi}_i|} \right| U_{N'\alpha'_i}(\rho) \\ &- \frac{Z}{\rho |(\beta_i \sin \phi_i) \hat{\eta}_i + (\frac{1}{2\beta_i} \cos \phi_i) \hat{\xi}_i|} \left| N'\alpha'_i > U_{N'\alpha'_i}(\rho) \right| \end{aligned} \right\} = 0 \quad (15)$$

Mass of the particles involved in the present calculation is partly taken from [1-2, 28-30, 68-69]. A straight forward evaluation of the matrix elements of last two terms in eq.(15) would be prohibitively involved both for analytical reduction to a computationally feasible form, as well as for the numerical calculation. Furthermore, the numerical calculation would be both inaccurate and time consuming. Application of RRC greatly simplifies the calculation, since in the partitions k and j , the third and fourth terms inside ket-bra $\langle \rangle$ notation in eq.(15) is reduced to $\frac{Z\beta_k}{\rho \cos \phi_k}$ and $\frac{Z\beta_j}{\rho \cos \phi_j}$ respectively. In the case of two-electron ions,

$$\beta_j = \beta_k = \left[1 - \frac{m^2}{(m_C + m)^2} \right]^{\frac{1}{4}} \quad (16)$$

In the case of a heavy nucleus, $m_C \gg m$ and $\beta_i \approx \frac{1}{\sqrt{2}}$, $\beta_j = \beta_k \simeq 1$.

We expand the three-body relative wave function in the complete set of HH appropriate to the partition i according to eq.(5). For the low-lying $^1,^3\text{S}$ -states of two-electron systems the total orbital angular momentum, $L=0$. Consequently $l_{\xi_i} = l_{\eta_i}$. Hence the set of quantum numbers represented by α_i is $\{l_{\xi_i}, l_{\xi_i}, 0, 0\}$ and the quantum numbers $\{N\alpha_i\}$ can be represented by $\{Nl_{\xi_i}\}$ only. Furthermore for $S=0$, spin part of the two-electron wave function is anti-symmetric, hence the space part of the wave function must be symmetric under exchange of two electrons which allows only even values of l_{ξ_i} ($\leq N/2$). On the other hand for $S=1$, spin part of the wave function is symmetric, hence space part of the wave function must be anti-symmetric under the exchange of the two electrons

which allows only odd values of l_{ξ_i} ($\leq N/2$) are to be considered. Corresponding HH is then given by [65]

$$\left. \begin{aligned} \mathcal{H}_{N\alpha_i}(\Omega_i) &\equiv \mathcal{H}_{Nl_{\xi_i}l_{\xi_i}00}(\Omega_i) \\ &= {}^{(2)}P_N^{l_{\xi_i}l_{\xi_i}}(\phi_i) \left[Y_{l_{\xi_i}m_{\xi_i}}(\theta_{\xi_i}, \phi_{\xi_i}) Y_{l_{\xi_i}-m_{\xi_i}}(\theta_{\xi_i}, \phi_{\xi_i}) \right]_{00} \\ &\quad \begin{array}{l} N \text{ even and } l_{\xi_i} = 0, 2, 4, \dots, \leq N/2 \text{ for } {}^1S \text{ states;} \\ l_{\xi_i} = 1, 3, 5, \dots, \leq N/2 \text{ for } {}^3S \text{ states} \end{array} \end{aligned} \right\} \quad (17)$$

The matrix element of the two electron repulsion term in our chosen partition i is

$$\begin{aligned} \langle N'l'_{\xi_i} | \frac{\beta_i}{\rho \cos \phi_i} | Nl_{\xi_i} \rangle &= \frac{\beta_i}{\rho} \delta_{l'_{\xi_i}, l_{\xi_i}} \int_0^{\pi/2} {}^{(2)}P_{K'}^{l_{\xi_i}l_{\xi_i}}(\phi) \\ &\quad \times {}^{(2)}P_N^{l_{\xi_i}l_{\xi_i}}(\phi) \sin^2 \phi \cos \phi d\phi \end{aligned} \quad (18)$$

in which suffix i on ϕ has been dropped deliberately as it is only a variable of integration. Similarly the matrix element of the third term of the total potential in eq.(15) in the partition k is

$$\begin{aligned} \langle N'l'_{\xi_k} | \frac{\beta_k}{\rho \cos \phi_k} | Nl_{\xi_k} \rangle &= \frac{\beta_k}{\rho} \delta_{l'_{\xi_k}, l_{\xi_k}} \int_0^{\pi/2} {}^{(2)}P_{N'}^{l_{\xi_k}l_{\xi_k}}(\phi) \\ &\quad \times {}^{(2)}P_N^{l_{\xi_k}l_{\xi_k}}(\phi) \sin^2 \phi \cos \phi d\phi \end{aligned} \quad (19)$$

A similar relation holds for the matrix element of the last term of the total potential in eq. (15) in the partition j . Eq.(18) and (19) show that the matrix elements are essentially the same in the respective partitions, although l_{ξ_k} and l_{ξ_j} are not restricted to only even or odd integer values. Each involves only a single, one dimensional integral to be performed numerically. Using eq.(12), matrix elements of the third and fourth terms of the total potential in eq.(15) in the partition i become

$$\begin{aligned} \langle N'l'_{\xi_i} | \frac{Z}{r_{ij}} | Nl_{\xi_i} \rangle &= \sum_{l_{\xi_k}} \langle l_{\xi_k}l_{\xi_k} | l'_{\xi_i}l'_{\xi_i} \rangle_{K'0} \langle l_{\xi_k}l_{\xi_k} | l_{\xi_i}l_{\xi_i} \rangle_{N0} \\ &\quad \langle K'l_{\xi_k} | \frac{Z\beta_k}{\rho \cos \phi_k} | Kl_{\xi_k} \rangle. \end{aligned} \quad (20)$$

and

$$\begin{aligned} \langle N'l'_{\xi_i} | \frac{Z}{r_{ik}} | Nl_{\xi_i} \rangle &= \sum_{l_{\xi_j}} \langle l_{\xi_j}l_{\xi_j} | l'_{\xi_i}l'_{\xi_i} \rangle_{N'0} \langle l_{\xi_j}l_{\xi_j} | l_{\xi_i}l_{\xi_i} \rangle_{N0} \\ &\quad \langle N'l_{\xi_j} | \frac{Z\beta_j}{\rho \cos \phi_j} | Nl_{\xi_j} \rangle. \end{aligned} \quad (21)$$

In eq.(20) and (21) sums over l'_{ξ_k} and l'_{ξ_j} respectively have been performed using the Kronecker - δ 's in eq.(19) and a similar one with suffix k replaced by suffix j . Thus the calculation of the matrix elements of all the interactions become practically simple and easy to handle numerically.

Although the rate of convergence of HH expansion is reasonably fast [70] for short-range interaction potentials [67, 70-71], the same cannot be claimed for long-range coulomb potentials. So to achieve desired convergence, large enough N_m value is to be included in the calculation. In the case of singlet spin ($S=0$) states, if all N values up to a maximum of N_m are retained in the HH expansion then the number of such basis function is

$$N_B = \begin{cases} \left(\frac{N_m}{4} + 1 \right)^2 & \text{if } \frac{N_m}{2} \text{ is even} \\ \frac{(\frac{N_m}{2} + 1)(\frac{N_m}{2} + 3)}{4} & \text{if } \frac{N_m}{2} \text{ is odd.} \end{cases} \quad (22)$$

and that for the triplet spin state (S=1) is

$$N_B = \begin{cases} \left(\frac{N_m}{4}\right)\left(\frac{N_m}{4} + 1\right) & \text{if } \frac{N_m}{2} \text{ is even} \\ \left(\frac{N_m+2}{4}\right)^2 & \text{if } \frac{N_m}{2} \text{ is odd.} \end{cases} \quad (23)$$

It can be checked from eq.(22) and eq. (23) respectively, that the number of basis states (N_B) and hence the size of CDE {eq.(6)} increases rapidly as N_m increases. For example, for $N_m = 96$ one has to solve 625 CDE for singlet spin and 600 CDE for the triplet spin configuration respectively which lead the calculation towards instability. We used dual-core based desktop computer for the present calculation and could solve only up to $N_m = 28$ reliably. The calculated binding energy (B_{N_m}) for values of N_m up to 28 are presented in columns 2 -10 of Table I for few low-lying $^{1,3}\text{S}$ -states of two-electron Coulombic systems like neutral helium and highly ionized radon Rn^{84+} and that for Rb^{35+} is presented in Table 3. The energies for still higher $N_m(> 28)$ may be obtained by following an extrapolation theorem suggested by Schneider [72] as discussed below. According to the theorem on convergence of HH one may expect following relation to hold for coulomb interaction:

$$(N_m + y)^4 \Delta B_{N_m} = C, \quad (24)$$

where

$$\Delta B_{N_m} = E_{N_m+4} - B_{N_m} \quad (25)$$

and y, C are constants. If one obtains y and C by solving eq.(24) for $N_m=16$ and 20 and uses eq.(24) to estimate the BE for $N_m = 28$, he finds that the estimated BE agrees fairly well with the BE actually calculated by solving CDE with $N_m = 28$. In this way one may verify that eq.(24) is well obeyed. For the converged extrapolated BE ($=B_{con} = B_{N_M}$), we calculated the constants y and C from eq.(24) by least square fitting B_{N_m} obtained by solving the CDE for $N_m = 0, 4, 8, \dots, \text{up to } 28$. With these values of y and C the extrapolated energies calculated by eq.(24) for larger $N_m (>28)$ are presented in columns 2-10 of Table 2. We select a value of $N_m(= N_M)$ for which ΔB_{N_m} is of the same order as the overall numerical error (ϵ) in the calculation of B_{N_m} with $N_m \leq 28$. Since, for any $N_m > N_M$, the correction ΔB_{N_M} will be smaller than ϵ and hence unreliable due to the finite numerical precision in solving the CDE. We estimated ϵ to be about 4×10^{-5} for a double precision calculation using dual-core based personal computer. The corresponding extrapolated results are presented in bold in column 4 of Table 4 and in columns 4 & 7 of Tables 5-7 together with some other results including the experimental ones for the low-lying $^{1,3}\text{S}$ -states wherever available. The term *exact* as the subscript of E in the 5th column of Table 5 refers to the results which were obtained by highly accurate variational procedures that involved very large numbers of linear and non-linear parameters [1-2,28-30]. The calculated energies for the low-lying bound 1,3 states for systems of different nuclear charge Z using data presented in column 3 of Table 4 and columns 3, 4 of Table 5-7 have been plotted in Figure 2 to see how the binding energies of the corresponding states depend on Z. To study the dependence of the convergence trend of calculated energy on Z, the difference in energy $\Delta B = B(N_m + 4) - B(N_m)$ is plotted in Figure 3 for few cases of different Z. Using the calculated energy data presented in Table 3 we have plotted Figures 4 and 5 to study the variation of the binding energy B and the quantity ΔB with

increase in N_m for ${}^\infty\text{Rb}^{84+}$. The convergence trend in energy can be checked by gradually increasing N_m values in suitable steps and comparing the energy difference $\Delta B = B(N+dN) - B(N)$ with that obtained in the previous step. By analysis of the calculated energy data presented in Table 1, it can be said that the energy of the lowest S-states in the lightest atom under consideration converges much faster than others with respect to the increase in N_m values. This trend of convergence with respect to the increasing N_m is slowed down gradually which can be viewed in two ways: (I) with respect to the increase in the level of excitation keeping nuclear charge number Z fixed and (II) with respect to the increase in the nuclear charge number (Z) for a particular level of excitation. For justifying our forgoing remarks -(I) we may compare the convergence trend in energy with respect to N_m for 2^3S and 4^3S states of neutral helium He ($Z=2$) or for the corresponding states of highly ionized radon Rn^{84+} ($Z=86$) by estimating and comparing the energy difference $\Delta B = B(N_m = 28) - B(N_m = 24)$ using the data presented in columns 4, 6 or those presented in columns 9, 11 of Table 1. These estimates for 2^3S and 4^3S states of neutral helium (He) are 0.0244au, 0.0660au and those for Rn^{84+} are 31.840au, 117.416au respectively thereby justifying our forgoing remarks -(I). Similar trends can also be seen in Figure 5 drawn for Rb^{35+} as representative case using data of Table 3. For the justification of our remarks -(II), we may compare the convergence trend in energy with respect to N_m for 4^1S state of neutral helium He ($Z=2$), positively charged rubidium Rb^{35+} ($Z=37$) and highly charged radon Rn^{84+} ($Z=86$) by estimating energy difference $\Delta B = B(N_m = 28) - B(N_m = 24)$ using the data presented in column 5 of Table 1, in column 7 of Table 3 and in column 10 of Table 1 respectively and compare them. And these estimates for 4^1S state of He , Rb^{35+} , Rn^{84+} are 0.0681au, 19.220au and 102.152au respectively thereby justifying our remarks -(II). Similar results can also be found for remaining levels of excitation using data presented in Table 1-3. This trend of convergence of energy is also demonstrated in Figure 3 for few low-lying $1,3\text{S}$ states of Rb^{35+} and Rn^{84+} respectively as representative cases. Furthermore it could also be noted that, although, the direct evaluation of the matrix element of $\frac{1}{r_{ij}}$ is possible in the partition i by the method of ref. [66], it is not possible for an interaction other than Coulombic or harmonic oscillator type. For an arbitrary shape of interaction potential, a direct calculation of the matrix element of the potential will involve five dimensional angular integrations which make the calculation very time consuming and leaves door open for inaccuracies to creep in easily. Hence the use of RRC for quick and accurate computation of energy in such cases becomes inevitable.

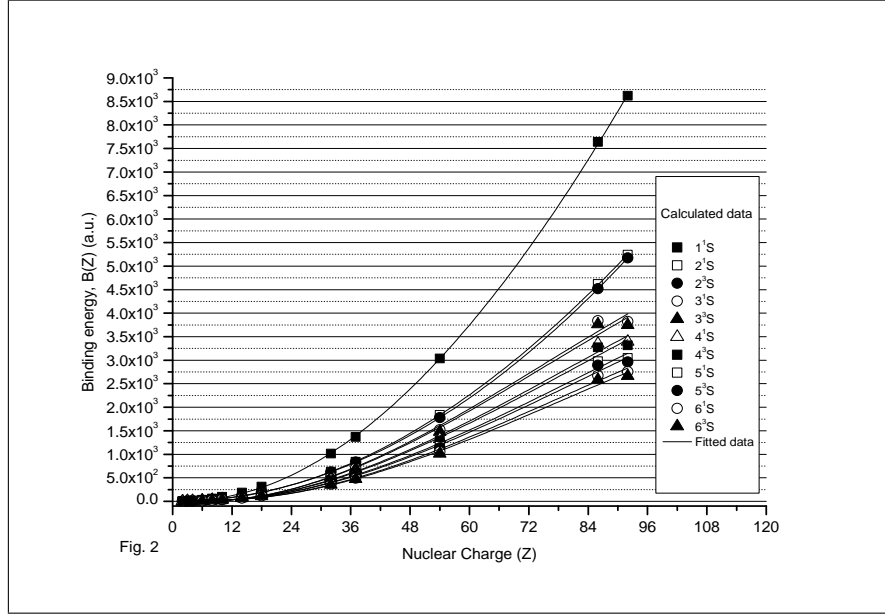


Figure 2: Dependence of the energy, $B(=-E)$ of the low-lying bound $1,3S$ -states of helium like Coulombic three-body system $\infty X^{(Z-2)+}$ ($X=\text{He, Li, Be, C, etc.}$) on the increase in nuclear charge Z . [Data source: Table 4-7]

One may see from Figure 2, that the calculated energy increases gradually with the increase in the charge number (Z) of the nuclear core of helium like Coulombic three-body systems $\infty X^{(Z-2)+}$ ($X=\text{He, Li, Be, C, ..., U}$). An approximate value of the energy of the low-lying bound $1,3S$ -states of any two-electron three-body system with a given Z can be estimated following empirical formula using the appropriate set of values of parameters p_0, p_1, p_2, p_3 recorded in Table 8

$$B(Z) = \sum_{j=0}^3 p_j Z^j \quad (26)$$

The values of the parameters p_0, p_1, p_2, p_3 presented in Table 8 are obtained by fitting the calculated energy data presented in Table 4 to Table 7 for the low-lying bound $1,3S$ -states of two-electron Coulombic three-body systems having nuclear charge (Z) in the range $Z=2$ to $Z=92$.

Figure 3 indicates that the rate of convergence in energy with respect to the gradual increase in the size of the basis states N_m in the case of Rn^{84+} ($Z=86$) is slower than that for Rb^{35+} ($Z=37$). This convergence trend can be checked by observing the relative decrement in the height of the bars corresponding to a particular level of excitation of Rb^{35+} and Rn^{84+} and comparing them with respect to gradually increasing values of N_m . For example, the height of the extreme left bar representing 1^1S state of Rb^{35+} decreases quicker than the height of the bar on its adjacent right representing 1^1S state of Rn^{84+} with increasing values of N_m . Similar observations hold for other quantum states (or levels of excitation) of the systems.

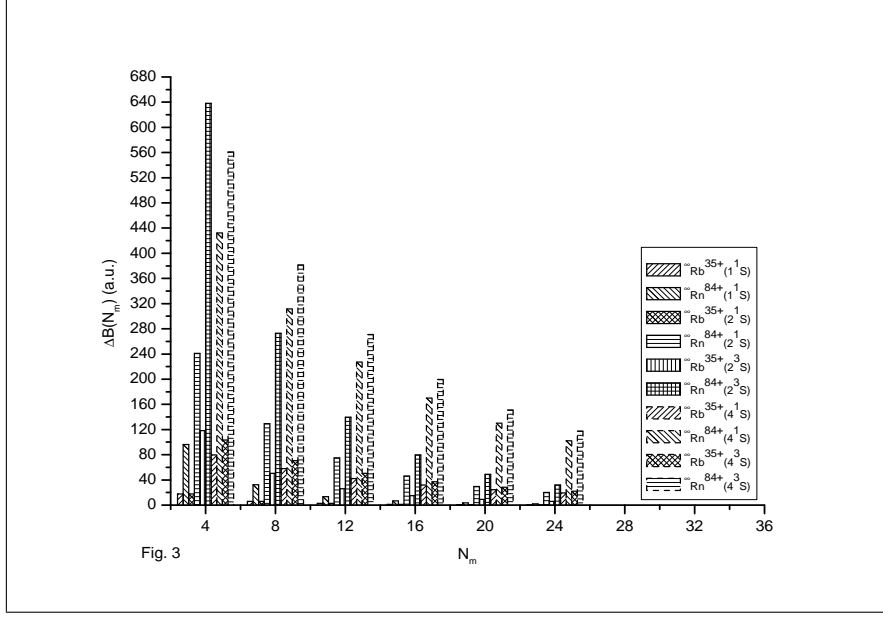


Figure 3: Dependence of the energy difference $\Delta B = B(N_m + 4) - B(N_m)$ on the increase in N_m for few low-lying bound $1,3S$ -states of helium like Coulombic three-body systems having different nuclear core charge Z . [Data source: Table 1 & 3]

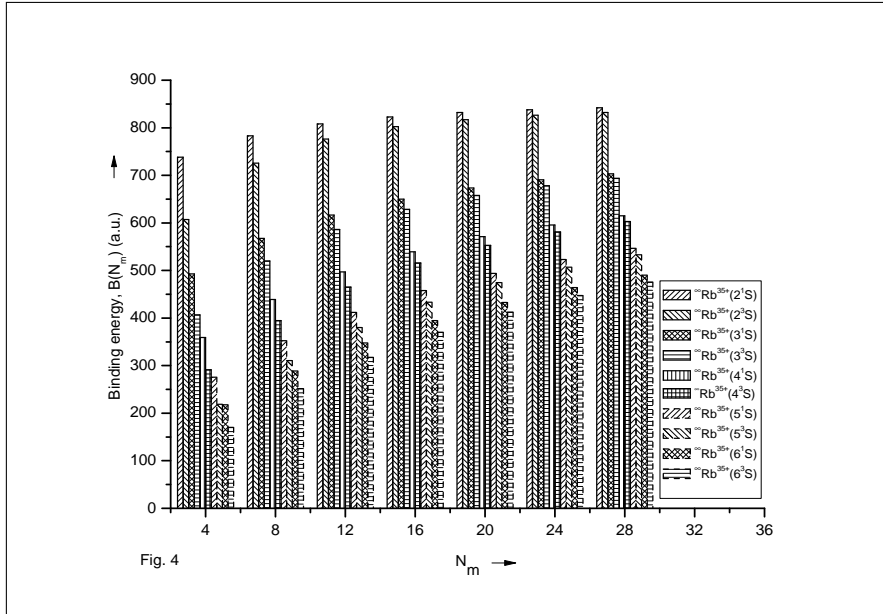


Figure 4: Dependence of the energy B ($= -E$) on the increase in N_m for few low-lying bound $1,3S$ -states of ${}^\infty\text{Rb}^{35+}$ ion. [Data source: Table 3]

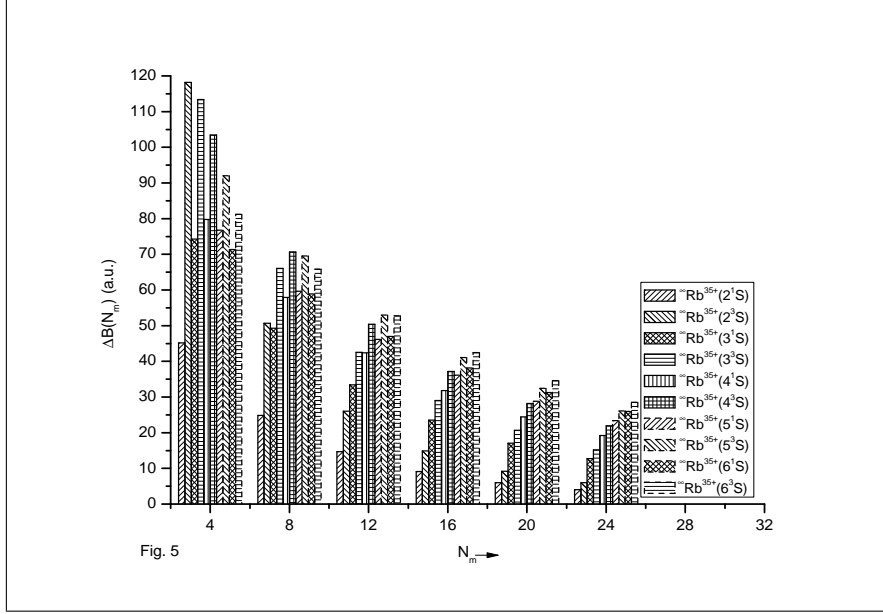


Figure 5: Dependence of the energy difference $\Delta B = B(N_m + 4) - B(N_m)$ on the increase in N_m for few low-lying bound $1,3S$ -states of ∞Rb^{35+} ion. [Data source: Table 3]

Further we have plotted in Figures 4 and 5 the variation of binding energy B , and the quantity ΔB against N_m for different low-lying bound $1,3S$ -states of Rb^{35+} ion as a representative case to study the convergence trend of energy of the low-lying bound S -states of a system with fixed Z using the data of Table 3. And it is observed from Figures 4 and 5, that the energies obtained for relatively lower levels converges earlier than the higher ones. Finally in Tables 4-7, the energies of the low-lying bound $1,3S$ -states for several Coulombic three-body systems obtained by solving the truncated set of coupled differential equations by the renormalized Numerov method [48] in the framework of HHE aided by RRC, have been compared with the ones of the literature.

4 Conclusion

In conclusion, we note that the use of RRC in HHE method becomes inevitable for the solution of the three-body Schrödinger equation, if the inter-particle interaction is other than Coulomb or harmonic type. Hence these coefficients are of immense importance for any type of interaction involved in three-body calculation. However in Tables 4, the calculated energy of the bound $1,3S$ -state at $N_m=28$ in most cases are smaller than those listed in column 5 & 6. This is due to the eventual truncation of expansion basis to a maximum value of N up to $N_m=28$ due to computer memory limitation. However, one may extrapolate the calculated energy values for $N_m=0, 4, 8, \dots$ etc. to get the solution for still higher $N_m > 28$ which have been described in the previous section and the corresponding extrapolated data (for $N_m > 28$) have been demonstrated in

Table 2 for few low-lying S-states of He and Rn as representative cases. The extrapolated energy values (at $N_m=N_M$) are listed in bold in the 4th column of Table 4 and in columns 4,7 of Tables 5-7. The extrapolated energies agree fairly well with the corresponding exact values found in the literature. One of the important aspect of RRC's are that they are independent of r , and need to be calculated once only and stored, resulting in an economic and highly efficient numerical computation. Finally we note that by the present method one can describe the Coulombic three-body systems in a very systematic and elegant manner with assured convergence. The method could also be applied to more complex Coulombic or nuclear systems by the proper choice of inter-particle potentials and expansion basis.

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6 Figure caption

Figure 1. Particle label scheme for general three-body system and choice of Jacobi coordinates in the i^{th} partition.

Figure 2. Dependence of the energy, $B(=-E)$ of the low-lying bound $^{1,3}S$ -states of helium like Coulombic three-body system $^{\infty}X^{(Z-2)+}$ ($X=He, Li, Be, C$, etc.) on the increase in nuclear charge Z . [Data source: Table 4-7]

Figure 3. Dependence of the energy difference $\Delta B = B(N_m + 4) - B(N_m)$ on the increase in N_m for few low-lying bound $^{1,3}S$ -states of helium like Coulombic three-body systems having different nuclear core charge Z . [Data source: Table 1 & 3]

Figure 4. Dependence of the energy $B(=-E)$ on the increase in N_m for few low-lying bound $^{1,3}S$ -states of $^{\infty}Rb^{35+}$ ion. [Data source: Table 3]

Fig. 5. Dependence of the energy difference $\Delta B = B(N_m + 4) - B(N_m)$ on the increase in N_m for few low-lying bound $^{1,3}S$ -states of $^{\infty}Rb^{35+}$ ion. [Data source: Table 3]

7 Tables

Table 1. Convergence trend of the energy calculated for few low-lying bound $^{1,3}S$ -states of neutral helium ($^{\infty}\text{He}$) and highly charged radon ($^{\infty}\text{Rn}^{84+}$) for increasing N_m .

Binding energy ($=B_{N_m}$ for $N = N_m$) in atomic unit (a.u.) in the $^{1,3}S$ state of:										
N_m	He_{1^1S}	He_{2^1S}	He_{2^3S}	He_{4^1S}	He_{4^3S}	$\text{Rn}_{1^1S}^{84+}$	$\text{Rn}_{2^1S}^{84+}$	$\text{Rn}_{2^3S}^{84+}$	$\text{Rn}_{4^1S}^{84+}$	$\text{Rn}_{4^3S}^{84+}$
0	2.5000	1.2755		0.5109		7065.857	3573.695		1438.793	
4	2.7844	1.5993	1.3725	0.8080	0.6551	7482.252	4076.054	3309.720	1977.548	1591.887
8	2.8562	1.7715	1.7268	1.0414	0.9524	7578.353	4316.945	3947.931	2410.031	2152.732
12	2.8760	1.8785	1.8893	1.2133	1.1600	7610.622	4446.135	4220.691	2721.692	2534.140
16	2.8875	1.9477	1.9788	1.3411	1.3106	7624.146	4520.970	4360.459	2948.823	2805.175
20	2.8936	1.9946	2.0332	1.4378	1.4227	7630.732	4567.020	4440.276	3118.704	3004.615
24	2.8970	2.0275	2.0687	1.5125	1.5080	7634.293	4596.738	4489.347	3249.001	3155.771
28	2.8990	2.0541	2.0931	1.5706	1.5740	7636.379	4616.679	4521.187	3351.153	3273.187

Table 2. Convergence trend of the extrapolated energy obtained for few low-lying bound $^{1,3}S$ -states of helium ($^{\infty}\text{He}$) and ionized radon ($^{\infty}\text{Rn}^{84+}$) for increasing N_m .

Binding energy ($=B_{N_m}$ for $N = N_m$) in atomic unit (a.u.) in the $^{1,3}S$ state of:										
N_m	He_{1^1S}	He_{2^1S}	He_{2^3S}	He_{4^1S}	He_{4^3S}	$\text{Rn}_{1^1S}^{84+}$	$\text{Rn}_{2^1S}^{84+}$	$\text{Rn}_{2^3S}^{84+}$	$\text{Rn}_{4^1S}^{84+}$	$\text{Rn}_{4^3S}^{84+}$
32	2.9003	2.0722	2.1091	1.6184	1.6255	7637.729	4630.917	4542.088	3434.018	3363.887
36	2.9011	2.0858	2.1206	1.6571	1.6665	7638.621	4641.212	4556.607	3500.912	3434.194
40	2.9017	2.0963	2.1289	1.6889	1.6995	7639.235	4648.840	4567.006	3555.503	3491.030
44	2.9021	2.1045	2.1351	1.7152	1.7264	7638.670	4654.612	4574.646	3600.493	3537.043
48	2.90240	2.1110	2.1399	1.7371	1.7485	7639.988	4659.058	4580.386	3637.905	3574.690
52	2.9026	2.1162	2.1436	1.7556	1.7668	7640.224	4662.539	4584.781	3669.268	3605.789
56	2.9028	2.1205	2.1465	1.7712	1.7822	7640.405	4665.303	4588.203	3695.757	3631.704
60	2.9029	2.1240	2.1488	1.7845	1.7951	7640.545	4667.526	4590.906	3718.283	3653.472
64	2.9031	2.1267	2.1507	1.7960	1.8061	7640.655	4669.333	4593.071	3737.560	3671.889
68	2.9031	2.1293	2.1522	1.8059	1.8155	7640.742	4670.817	4594.824	3754.154	3687.577
72	2.9032	2.1313	2.1535	1.8144	1.8236	7640.813	4672.048	4596.259	3768.515	3701.022
76	2.9033	2.1330	2.1545	1.8219	1.8305	7640.871	4673.077	4597.445	3781.006	3712.612
80	2.9033	2.1345	2.1554	1.8284	1.8366	7640.918	4673.944	4598.434	3791.923	3722.656
84	2.9034	2.1358	2.1561	1.8342	1.8419	7640.958	4674.680	4599.265	3801.506	3731.402
88	2.9034	2.1369	2.1568	1.8393	1.8465	7640.991	4675.308	4599.968	3809.952	3739.055
92	2.9034	2.1378	2.1573	1.8438	1.8506	7641.019	4675.848	4600.567	3817.425	3745.780
96	2.9034	2.1386	2.1578	1.8478	1.8542	7641.043	4676.314	4601.081	3824.061	3751.713
100	2.9035	2.1394	2.1582	1.8513	1.8575	7641.063	4676.719	4601.524	3829.975	3756.967
104	2.9035	2.1400	2.1585	1.8545	1.8603	7641.081	4677.072	4601.908	3835.261	3761.638
108	2.9035	2.1406	2.1588	1.8574	1.8629	7641.096	4677.382	4602.242	3840.001	3765.803
112	2.9035	2.1411	2.1591	1.8600	1.8651	7641.109	4677.654	4602.535	3844.264	3769.529
116	2.9035	2.1415	2.1593	1.8623	1.8672	7641.121	4677.895	4602.792	3848.108	3772.873
120	2.9035	2.1419	2.1596	1.8644	1.8690	7641.131	4678.109	4603.019	3851.584	3775.882
124	2.9035	2.1423	2.1597	1.8664	1.8707	7641.140	4678.299	4603.220	3854.734	3778.597
128	2.9035	2.1426	2.1599	1.8681	1.8722	7641.148	4678.469	4603.399	3857.596	3781.054
132	2.9036	2.1429	2.1601	1.8697	1.8736	7641.155	4678.621	4603.558	3860.202	3783.282
136	2.9036	2.1431	2.1602	1.8711	1.8749	7641.161	4678.758	4603.701	3862.579	3785.307
140	2.9036	2.1434	2.1603	1.8725	1.8760	7641.167	4678.881	4603.829	3864.754	3787.152
144	2.9036	2.1436	2.1604	1.8737	1.8770	7641.172	4678.992	4603.944	3866.746	3788.837
148	2.9036	2.1438	2.1605	1.8748	1.8780	7641.176	4679.093	4604.048	3868.574	3790.378
152	2.9036	2.1439	2.1606	1.8758	1.8789	7641.180	4679.184	4604.143	3870.255	3791.790
156	2.9036	2.1441	2.1607	1.8768	1.8797	7641.184	4679.267	4604.228	3871.804	3793.087
160	2.9036	2.1442	2.1608	1.8777	1.8804	7641.187	4679.343	4604.305	3873.233	3794.281
164	2.9036	2.1444	2.1608	1.8785	1.8811	7641.190	4679.412	4604.376	3874.553	3795.380
168	2.9036	2.1445	2.1609	1.8792	1.8817	7641.193	4679.476	4604.441	3875.775	3796.395
172	2.9036	2.1446	2.1609	1.8799	1.8823	7641.195	4679.534	4604.500	3876.908	3797.334
176	2.9036	2.1447	2.1610	1.8806	1.8829	7641.198	4679.587	4604.554	3877.959	3798.202
180	2.9036	2.1448	2.1610	1.8812	1.8834	7641.200	4679.637	4604.604	3878.937	3799.007
184	2.9036	2.1449	2.1611	1.8817	1.8838	7641.202	4679.682	4604.649	3879.846	3799.756
188	2.9036	2.1450	2.1611	1.8823	1.8843	7641.203	4679.724	4604.692	3880.694	3800.451
192	2.9036	2.1451	2.1611	1.8827	1.8847	7641.205	4679.763	4604.730	3881.485	3801.099
196	2.9036	2.1451	2.1612	1.8832	1.8851	7641.207	4679.799	4604.766	3882.223	3801.702
200	2.9036	2.1452	2.1612	1.8836	1.8854	7641.208	4679.832	4604.800	3882.914	3802.266
204	2.9036	2.1453	2.1613	1.8840	1.8857	7641.209	4679.863	4604.831	3883.561	3802.792
208	2.9036	2.1453	2.1613	1.8844	1.8860	7641.211	4679.892	4604.859	3884.167	3803.284
212	2.9036	2.1454	2.1613	1.8848	1.8863	7641.212	4679.919	4604.886	3884.735	3803.745
216	2.9036	2.1454	2.1613	1.8851	1.8866	7641.213	4679.944	4604.911	3885.269	3804.177
220	2.9036	2.1455	2.1614	1.8854	1.8869	7641.214	4679.967	4604.934	3885.771	3804.583

Table 3. Pattern of convergence of the calculated energy (in atomic unit) for the low-lying bound $^{1,3}\text{S}$ -states $^{\infty}\text{Rb}^{35+}$ ion for increasing N_m .

N_m	B(1^1S)	B(2^1S)	B(2^3S)	B(3^1S)	B(2^3S)	B(4^1S)	B(4^3S)	B(5^1S)	B(5^3S)
0	1264.570	645.919		389.957		260.452		186.103	
4	1340.648	738.134	607.378	493.011	406.631	359.347	291.160	275.378	218.704
8	1358.438	783.281	725.557	567.303	520.017	439.137	394.568	352.145	310.756
12	1364.548	808.142	776.213	616.614	586.098	497.042	465.246	411.821	380.261
16	1367.139	822.797	802.266	650.037	628.633	539.433	515.660	457.947	433.232
20	1368.412	831.933	817.185	673.538	657.660	571.245	552.834	494.105	474.305
24	1369.104	837.886	826.380	690.615	678.330	595.707	581.043	522.943	506.763
28	1369.511	841.914	832.357	703.368	693.539	614.927	602.972	546.324	532.871

Table 4. Comparison of calculated energy for the low-lying bound $1,3S(L=0)$ -states of helium and helium like Coluombic three-body systems with the ones of the literature.

System	State	Binding energy, B ($=B_{N_m}$ for $N = N_m$) in atomic unit (a.u.)			
		$B_{N_m=28}$	$B_{N_m=N_M}$	E_{exact}	Other sources
^3He	1^1S	2.89845295	2.90324338	2.90316721 [35]	2.90051530 [1]
	2^1S	2.05107241	2.13814412	2.14558192 [35]	2.14501773 [1]
	2^3S	2.09269897	2.16138053	2.17483231 [35]	2.17454273 [1]
	3^1S	1.78731919	2.00852819	2.06089652 [35]	2.06069722 [1]
	3^3S	1.80010572	2.00295712	2.06831238 [35]	2.06820440 [1]
	4^1S	1.57029931	1.88975703	2.03321657 [35]	2.02623837 [1]
	4^3S	1.57365954	1.89174046	2.03614146 [35]	2.03156807 [1]
	1^1S	2.89859016	2.90338079	2.90330456 [35]	2.90065336 [1]
^4He				2.90372440 [24]	2.90368830 [14]
	2^1S	2.05116527	2.13824141	2.14567859 [35]	2.14511445 [1]
	2^3S	2.09279342	2.16147778	2.17493019 [35]	2.17464057 [1]
	3^1S	1.78740060	2.00862130	2.06098908 [35]	2.06078978 [1]
	3^3S	1.80018701	2.00304736	2.06840524 [35]	2.06829724 [1]
	4^1S	1.57037897	1.88986615	2.03330782 [35]	2.02633010 [1]
	4^3S	1.57373604	1.89184097	2.03623283 [35]	2.03165943 [1]
	1^1S	2.89900954	2.90380076	2.90372438 [35]	2.90107544 [1]
				2.90372438 [22]	
	2^1S	2.05414493	2.14642285	2.14597405 [35]	2.14541020 [1]
	2^3S	2.09308211	2.16177503	2.17522938 [35]	2.17493966 [1]
	3^1S	1.78764955	2.01000443	2.06127199 [35]	2.06107284 [1]
$^\infty\text{He}$	3^3S	1.80043551	2.00332324	2.06868907 [35]	2.06858102 [1]
	4^1S	1.57062240	1.89199576	2.03358672 [35]	2.02660791 [1]
	4^3S	1.57396988	1.89214821	2.03651208 [35]	2.03193872 [1]
	1^1S	7.27068287	7.27959321	7.27922302 [35]	7.27588119 [1]
	2^1S	4.88519501	5.03990504	-	5.03894691 [1]
	2^3S	4.96035893	5.09413803	-	5.10969189 [1]
	3^1S	4.21338221	4.67184315	-	4.73266048 [1]
	3^3S	4.22271122	4.64640852	-	4.75130451 [1]
	4^1S	3.72411106	4.48575388	-	4.62472771 [1]
	4^3S	3.70030123	4.43114605	-	4.63390581 [1]
	5^1S	3.32869817	4.39001212	-	-
	5^3S	3.28429267	4.31111429	-	-
$^6\text{Li}^+$	1^1S	7.27078128	7.27969173	7.27932152 [35]	7.20603060 [1]
	2^1S	4.88525904	5.03997129	-	5.03913196 [1]
	2^3S	4.96042382	5.09420455	-	5.10975862 [1]
	3^1S	4.21343739	4.67190463	-	4.73315062 [1]
	3^3S	4.22276636	4.64646894	-	4.75136656 [1]
	4^1S	3.724159	4.48581310	-	4.62641756 [1]
	4^3S	3.70034950	4.43120337	-	4.63396662 [1]
	5^1S	3.328742	4.39006911	-	-
	5^3S	3.28433555	4.31117021	-	-
	1^1S	7.27137265	7.28028376	7.27991341 [35]	7.27657671 [1]
	2^1S	4.88564379	5.04036937	7.27991341 [22]	7.27991341 [74]
	2^3S	4.96081374	5.09460425	5.04087674 [73]	5.03941025 [1]
				5.11072731 [73]	5.11015939 [1]
$^\infty\text{Li}^+$				5.11072737 [20]	
	3^1S	4.21376895	4.67227404	4.73375186 [73]	4.73309441 [1]
	3^3S	4.22309769	4.64683203	4.75207644 [73]	4.75173831 [1]
	4^1S	3.72445246	4.48616767	4.62977459 [73]	4.62515508 [1]
	4^3S	3.70063956	4.43154788	4.63713654 [73]	4.63433035 [1]
	5^1S	3.32900485	4.39042199	-	-
	5^3S	3.28459324	4.31150622	-	-

Table 5. Comparison of calculated energy for the low-lying bound $^1,^3S(L=0)$ -states of helium like Columbic three-body systems with the ones of the literature.

System	State	Binding energies B_{N_m} for $N = N_m$ in atomic unit for $^1,^3S$ - states				
		$B_{N_m=28}$	$B_{N_m=N_M}$	State	$B_{N_m=28}$	$B_{N_m=N_M}$
$^{10}\text{Be}^{2+}$	1^1S	13.64100542	13.65555317 13.6555662 [24] 13.6555322 [14]			
	2^1S	8.94911216	9.19161005	2^3S	9.05459257	9.27634522
	3^1S	7.66804423	8.44652588	3^3S	7.66497104	8.38910901
	4^1S	6.76103019	8.08313611	4^3S	6.70286146	7.97128862
	1^1S	13.64177142	13.65631993 13.65566238[22] 13.65566238[74]			
$^\infty\text{Be}^{2+}$	2^1S	8.94960223	9.19333838	2^3S	9.27685193	9.27685193 9.29716659 [20]
	3^1S	7.66846380	8.45124727	3^3S	7.66538960	8.38956578
	4^1S	6.76066022	8.08949853	4^3S	6.70322721	7.97172093
	5^1S	6.03494406	7.90747336	5^3S	5.94304043	7.74863876
$^{12}\text{C}^{4+}$	1^1S	32.37663926	32.40685560 32.4062466 [24] 32.4062132 [14]			
	2^1S	20.77005736	21.24818024	2^3S	20.92259034	21.38852080
	3^1S	17.66499856	19.33438639	3^3S	17.60913254	19.17442075
	4^1S	15.53267060	18.43106051	4^3S	15.36613898	18.15220701
	5^1S	13.84303207	17.96048254	5^3S	13.60727634	17.59965248
$^\infty\text{C}^{4+}$	1^1S	32.37814008	32.40835778 32.40624660[22] 32.40624660[73]			
	2^1S	20.77100359	21.25084519	2^3S	20.92354286	21.38949376 21.4207559 [20]
	3^1S	17.66580282	19.34319951	3^3S	17.60993325	19.17529100
	4^1S	15.53337831	18.44829391	4^3S	15.36683732	18.15302868
	5^1S	13.84366250	17.98746303	5^3S	13.60789448	17.60044649
$^{16}\text{O}^{6+}$	6^1S	12.44587479	17.78810696	6^3S	12.16585900	14.83317733
	1^1S	59.10834846	59.16004356 59.156 5951 [24] 59.1565622 [14]			
	2^1S	37.51773633	38.31230986	2^3S	37.69735366	38.49829459
	3^1S	31.77962231	34.67519168	3^3S	31.63349495	34.36036915
$^\infty\text{O}^{6+}$	4^1S	27.90383672	32.99044656	4^3S	27.57415238	32.46790039
	5^1S	24.84856668	32.10636657	5^3S	24.40313985	31.44020700
	6^1S	22.32748157	31.59904473	6^3S	21.80904495	30.92526993
	1^1S	59.11039341	59.16209025 59.15659512 [22] 59.15659512 [73]			
	2^1S	37.51901718	38.31361890	2^3S	37.69863997	38.49960746 38.54464732 [20]
$^{20}\text{Ne}^{8+}$	3^1S	31.78070668	34.67637674	3^3S	31.63457330	34.36153886
	4^1S	27.90478889	32.99157418	4^3S	27.57509196	32.46900346
	5^1S	24.84941473	32.10746357	5^3S	24.40397111	31.44127245
	6^1S	22.32824372	31.60009809	6^3S	21.80904495	30.98033807
	1^1S	93.83962679	93.92037567 93.9068065 [24] 93.9067737 [14]			
$^\infty\text{Ne}^{8+}$	2^1S	59.19300213	60.38347654	2^3S	59.37879471	60.60552089
	3^1S	50.01242982	54.46894570	3^3S	49.73801357	53.94690740
	4^1S	43.87450984	51.75982348	4^3S	43.32683791	50.91827229
	5^1S	39.05150768	50.33364370	5^3S	38.33024314	49.26976804
	1^1S	93.84221663	93.92117897 93.90680652 [22] 93.90680651 [73]			
	2^1S	59.19521811	60.38674068	2^3S	59.38041492	60.60717382 60.66864658 [20]
	3^1S	50.01379450	54.46665522	3^3S	50.01279450	53.94837663
	4^1S	43.87570737	51.76123767	4^3S	43.32801878	50.91965680
	5^1S	39.05257343	50.33501851	5^3S	38.33128755	49.27110500
	6^1S	35.07883941	49.78428221	6^3S	34.24708372	48.51818062

Table 6. Calculated energy for the low-lying bound $1,3S(L=0)$ -states of helium like Coluombic three-body systems for which reference values are not available.

System	State	Binding energies B_{N_m} for $N = N_m$ in atomic unit for $1,3S$ - states			
		$B_{N_m=28}$	$B_{N_m=N_M}$	State	$B_{N_m=28}$
$^{28}\text{Si}^{12+}$	1^1S	187.33623586	187.48697007		
	2^1S	117.34098803	119.56568139	2^3S	117.46178209
	3^1S	98.83846617	107.41844030	3^3S	98.18763000
	4^1S	86.61882068	101.92547321	4^3S	85.46630711
	5^1S	77.05326349	99.03169898	5^3S	75.57824630
$^{\infty}\text{Si}^{12+}$	1^1S	187.33991986	187.49065697		
	2^1S	117.34327599	119.56801338	2^3S	117.46407024
	3^1S	98.84039233	107.42053496	3^3S	98.18954155
	4^1S	86.62050862	101.93205784	4^3S	85.46797059
	5^1S	77.05476512	99.03362906	5^3S	75.57971705
	6^1S	69.18781295	97.87364713	6^3S	67.50779834
$^{40}\text{Ar}^{16+}$	1^1S	313.01347510	313.26016489		
	2^1S	195.25738776	198.82695786	2^3S	195.17203766
	3^1S	164.16773363	178.19631514	3^3S	162.95847989
	4^1S	143.78433327	168.94885492	4^3S	141.78501941
	5^1S	127.86367569	164.04660012	5^3S	125.35175859
$^{\infty}\text{Ar}^{16+}$	1^1S	313.01778694	313.26290079		
	2^1S	195.26005541	198.82967402	2^3S	195.17469823
	3^1S	164.16997440	178.19874736	3^3S	162.96070028
	4^1S	143.78629491	168.95116040	4^3S	141.78695094
	5^1S	127.86542065	164.04954287	5^3S	125.35346601
	6^1S	114.78563676	162.06610437	6^3S	111.94830964
$^{73}\text{Ge}^{30+}$	1^1S	1014.10495117	1014.83717742		
	2^1S	626.14203646	636.44668213	2^3S	621.72918896
	3^1S	524.12494015	567.05022289	3^3S	518.19512337
	4^1S	458.44873845	536.5722955	4^3S	450.57357075
	5^1S	407.40409820	520.37147652	5^3S	398.21122657
	6^1S	365.55993388	513.54614703	6^3S	355.54564542
$^{\infty}\text{Ge}^{30+}$	1^1S	1014.11284946	1014.84667354		
	2^1S	626.14680929	636.48612374	2^3S	621.73383114
	3^1S	524.12890560	567.25338865	3^3S	518.19899158
	4^1S	458.45220105	537.01104413	4^3S	450.57693397
	5^1S	407.40717276	521.09516457	5^3S	398.21419883
	6^1S	365.56269120	514.59886056	6^3S	355.54829917
$^{87}\text{Rb}^{35+}$	1^1S	1369.50177024	1370.45052824		
	2^1S	841.90857190	855.03234476	2^3S	832.35208572
	3^1S	703.36387502	759.78528149	3^3S	693.53427843
	4^1S	614.92316566	718.35308809	4^3S	602.96829556
	5^1S	546.32050458	696.26001256	5^3S	532.86744847
	6^1S	490.12802196	647.66171793	6^3S	475.75927472
$^{\infty}\text{Rb}^{35+}$	1^1S	1369.51091586	1370.46173546		
	2^1S	841.91402943	855.08151199	2^3S	832.357300378
	3^1S	703.36837784	760.05044604	3^3S	693.53862264
	4^1S	614.92709123	718.93145490	4^3S	602.97207243
	5^1S	546.32398759	696.26438420	5^3S	532.87078631
	6^1S	490.13114408	647.66577131	6^3S	475.76225492
$^{132}\text{Xe}^{52+}$	1^1S	3034.33032264	3036.10652657		
	2^1S	1835.73342239	1858.27421167	2^3S	1778.07908319
	3^1S	1520.10383171	1631.61384634	3^3S	1480.70025535
	4^1S	1326.34233956	1537.17817352	4^3S	1287.14195751
	5^1S	1177.30195319	1486.00908806	5^3S	1137.44912969
	6^1S	1055.62293041	1432.37045117	6^3S	1015.54664869
$^{\infty}\text{Xe}^{52+}$	1^1S	953.54597837	1365.70263779	7^3S	913.71200484
	1^1S	3034.34403549	3036.12024452		
	2^1S	1835.74140513	1858.28223928	2^3S	1778.08642782
	3^1S	1520.11029918	1631.62069230	3^3S	1480.70637251
	4^1S	1326.34795821	1537.18457058	4^3S	1287.14727680
	5^1S	1177.30693158	1486.01523381	5^3S	1137.45383214
	6^1S	1055.62738998	1432.37654976	6^3S	1015.55084882
	7^1S	953.55000451	1365.70825884	7^3S	913.71578525

Table 7. Calculated energy for the low-lying bound $^{1,3}S(L=0)$ -states of helium like Coluombic three-body systems for which reference values are not available.

System	State	Binding energies B_{N_m} for $N = N_m$ in atomic unit for $^{1,3}S$ - states			
		$B_{N_m=28}$	$B_{N_m=N_M}$	State	$B_{N_m=28}$ $B_{N_m=N_M}$
$^{222}\text{Rn}^{84+}$	1^1S	7636.36418198	7641.20543961		
	2^1S	4616.66857975	4680.19668342	2^3S	4521.17553625 4605.15844138
	3^1S	3837.15245292	4136.94140731	3^3S	3764.45017663 4058.24848136
	4^1S	3351.14526034	3893.40869622	4^3S	3273.17906922 3810.56957110
	5^1S	2976.42342407	3765.55061894	5^3S	2893.66454225 3671.16419665
	6^1S	2670.29151481	3593.02119421	6^3S	2584.74356269 3599.15482185
$^{\infty}\text{Rn}^{84+}$	1^1S	7636.37941153	7641.23108390		
	2^1S	4616.67861400	4680.41269088	2^3S	4521.18661942 4605.36483601
	3^1S	3837.16123452	4138.31425610	3^3S	3764.45941573 4059.27113623
	4^1S	3351.15302320	3896.39350957	4^3S	3273.18711492 3812.93142451
	5^1S	2976.43036542	3767.26785710	5^3S	2893.67166846 3675.21000221
	6^1S	2670.29777418	3599.22653486	6^3S	2584.74994153 3605.18235959
$^{238}\text{U}^{90+}$	1^1S	8618.00391229	8624.11550275		
	2^1S	5240.84978695	5319.84869467	2^3S	5174.74362888 5270.93881700
	3^1S	3819.79967898	4449.03430062	3^3S	3746.84431623 4360.91561578
	4^1S	3394.24156455	4305.79766260	4^3S	3312.84455557 4200.53296546
	5^1S	3046.23137764	3745.06335941	5^3S	2959.62690696 4182.50227889
	6^1S	2753.99116703	3988.35675960	6^3S	2664.58714689 3581.10905621
$^{\infty}\text{U}^{90+}$	1^1S	8618.01897182	8624.13058963		
	2^1S	5240.86018734	5319.85951984	2^3S	5174.75544789 5271.17435433
	3^1S	3819.80783330	4449.04422383	3^3S	3746.85290227 4360.92558161
	4^1S	3394.24887082	4305.80737378	4^3S	3312.85216467 4205.14588567
	5^1S	3046.23797736	3745.07101005	5^3S	2959.63372271 4190.22906381
	6^1S	2753.99716714	3988.36584661	6^3S	2664.59330043 3581.11748487

Table 8. Values of parameters involved in eq.(26) obtained by best fit of calculated energies.

State	Parameters (in atomic unit, 1au=27.12eV)			
	p_0	p_1	p_2	p_3
1^1S	28.8078	-7.33198	1.26212	-0.00178
2^1S	10.37378	-2.67664	0.71274	-7.02147E-4
2^3S	0.18499	-0.2216	0.61394	-1.53093E-6
3^1S	63.82991	-14.21409	1.04226	-0.00462
3^3S	59.93207	-13.24075	0.99848	-0.00435
4^1S	49.16737	-10.94696	0.85611	-0.00355
4^3S	46.22096	-10.21724	0.8198	-0.00335
5^1S	53.3078	-10.35107	0.76665	-0.00314
5^3S	49.91539	-9.62781	0.7305	-0.00294
6^1S	87.92359	-12.89187	0.76764	-0.0033
6^3S	82.89113	-11.97116	0.72684	-0.00307